

REMARKS/ARGUMENTS

Claims 3 and 4 are cancelled without prejudice. Claims 1, 2, 5, 6, and 7 have been amended to more clearly set forth that which the inventors claim as their invention. Claims 8 – 12 are new.

Examiner's Action:

Summarizing briefly, the Examiner has maintained the following rejections of the claims:
35 U.S.C § 112 first paragraph as failing to comply with the written description requirement.

“...The specification does not describe any molecules. There is no class, subclass or general structure of molecules being claimed. There is no specific core molecule to which the molecules are compared or combined. The claims now refer to molecules “which possess desired properties” with specifically naming any properties....The claims do not set forth any functional limitations which could effectively limit the underlying structure of the molecules being claimed...”

35 U.S.C. § 101 because the claimed invention is not supported by either a specific, substantial or credible asserted utility or a well established utility. ... The specification does not describe any molecules. There is no class, subclass or general structure of molecules being claimed. There is no specific core molecule to which the molecules are compared or combined. The claims now refer to molecules “which possess desired properties” with specifically naming any properties. The limitations regarding diversity sampling do not appear to limit the molecules themselves... No specific functions, activities, or use for the molecules are set forth in the claims. ...The claims do not set forth any structural

limitations which would limit the claimed molecules to a particular type or class. The claims do not set forth any functional limitation which could effectively limit the underlying structure of the molecules being claimed.

35 U.S.C. § 112 first paragraph Specifically, since the claimed invention is not supported by either a specific, substantial or credible asserted utility or a well established utility for the reasons set forth above, one skilled in the art clearly would not know how to use the claimed invention.

35 U.S.C. § 101 because the claimed invention is directed to non-statutory subject matter. ... However, the claims are drawn to products that have no specific structure, or function or even any tangible identity. Furthermore, the process steps in the claims do not end with assembled molecules, but with lists of reactants and cores that must be further acted upon to be used. ,, As set forth previously, the claims are drawn to nonfunctional descriptive material. ... These selected molecules are mere presentations of information or abstract ideas which have not been practically applied.

35 U.S.C. § 102(e) Applicant does not specifically address this rejection in the response..... However, the products of Agrafiotis are equivalent to the products being claimed absent evidence to the contrary.

Applicants' Response:

Applicants appreciate the examiner's comments and have again reviewed the Trilateral Project reports, particularly those concerning so called reach-through claims. The Reports define "reach-through claims" as "claims to future inventions based on currently disclosed inventions."

Trilateral Project B3b, Introduction. Applicants respectfully submit that the claims submitted in the present application are claims to present inventions. Applicants understand and appreciate the examiner's focus on the absence of specific molecular structures in the traditional sense. However, unlike the examples given in the Trilateral Reports, applicants' claims do not go to such things as molecules which could be discovered in a screening assay, or more generally to molecules having characteristics yet to be defined. On the contrary, applicants have disclosed methods for assembling groups of molecules having very specific and unique characteristics.

Applicants have amended the claims to further characterize the molecules which are claimed. Each of the molecules has unique and predetermined characteristics. In reviewing applicants' last response, applicants noticed that some of the characterizing limitations attributed to the claims by applicants were, perhaps, not as clearly spelled out in the claims as applicant understood them to be. Accordingly, the amended claims recite with more particularity the unique characteristics of the molecules set forth in each claim.

In addition to the remarks which follow, applicants incorporate in this response applicants' remarks in the prior response, and respectfully request the examiner to review those remarks again in light of the amended claims. For convenience of the examiner, those remarks are attached at the end of this response.

Response to 35 U.S.C. § 101 rejections.

"To comply with 35 U.S.C. § 101, the claimed invention must have at least one specific, substantial, and credible utility that is either asserted in the specification or well-established."

Trilateral Project B3b Report, page 22. Applicants submit that the claims directed to identifying

those molecules not having similar shapes and activities (claims 1 and 2) or to identifying those molecules having a shape and activity similar to a lead compound (claims 5 – 7) recite at least one specific, substantial, and credible utility that will be recognized by those skilled in the art. Further, the selected molecules do have specific structures and functions, depending upon how they were selected. For instance, the molecules of claims 5 – 7 have three dimensional structures and activities similar to that of a lead compound. In the drug discovery field, this is exactly the utility that is sought since lead compounds frequently either have undesirable side effects or low activity. By defining molecules with similar shapes and activities, the invention provides medicinal chemists with the opportunity to mine the molecules for more useful drugs.

The examiner also notes that “...the methods end with lists of reactants and cores which must be further acted upon to be used.” Applicants must respectfully disagree with the examiner’s reading of the claims. The claims end with either a list of the selected molecules being output or a list of the reagents and cores. Also, as taught in the specification, the lists of reactants and cores is equivalent to a list of the assembled products. Additionally, claim 7 notes in the preamble that the selection is made from “product molecules.”

The examiner has suggested that the claim language “could be made in a combinatorial synthesis of specified reactants and a common core” reflects the mere presentations of information or abstract ideas. Applicants note that in the amended claims submitted with the prior response, the language “could be made in a combinatorial synthesis of specified reactants and a common core” was changed to the more specific “derived from the combinatorial assembly of structural variations and common core. Along with the present amendments in which specific

utilities are highlighted, applicants respectfully submit that the claims should no longer be rejected under 35 U.S.C. § 101.

Response to 35 U.S.C. § 112 rejections:

“To comply with the written description requirement of 35 U.S.C. § 112, first paragraph, a patent specification must describe the claimed invention in sufficient detail that one skilled in the art can reasonably conclude that the inventor had possession of the claimed invention. ... Possession may be shown in a variety of ways including description of an actual reduction to practice...or by describing distinguishing identifying characteristics sufficient to show that the applicant was in possession of the claimed invention.” Trilateral Project B3b Report, page 22-23. As the examiner has pointed out, no specific molecules are described by the claims. Rather, the characteristics of the group/set of molecules selected – the relationship of the molecules to each other – is clearly set forth. The molecules covered by the claims would depend on the structural variations and cores present in the virtual library, and, in the case of claims 5 – 7, on the lead compound. However, applicants must respectfully disagree with the examiner that:

“No particular families or types of molecules are described in the claims. The claims do not set forth any structural limitations which would limit the claimed molecules to a particular type or class. The claims do not set forth any functional limitations which could effectively limit the underlying structure of the molecules being claimed.” Office Action, pages 2-3.

Applicants submit that the claims do set forth structural and activity (functional) limitations of the claimed molecules. Claims 1 and 2 require that the three dimensional structures and activities of

the molecules be dissimilar. Most obviously, claims 5 – 7 require that the three dimensional structures and activities of the molecules be similar to the three dimensional structure and activity of the lead compound. The fact that the claims define molecules in an assemblage of molecules where the molecules have specific relationships to each other does not mean that the written description requirement is not met. The claims are product-by-process claims and the products (molecules) must necessarily have the characteristics (as a group) determined for them by the process. The characteristics of the group of molecules are clearly described in the specification and claims. The generation of the molecular groups is fully enabled by the software code attached to the application. Applicants respectfully submit that the written description requirement is met.

The second 35 U.S.C. § 112 rejection parallels the 101 utility rejection. Since applicants have demonstrated at least one specific, substantial or credible asserted utility, applicants submit that one skilled in the art would clearly know how to use the claimed invention. Along these lines, it should be mentioned that those skilled in the art routinely define molecular assemblies by the manner in which they are generated.

Applicants respectfully submit that the claims should no longer be rejected under 35 U.S.C. § 112, first paragraph.

Response to 35 U.S.C. § 102(e) rejections:

The examiner has repeated the rejection first raised based on Agrafiotis. In particular the examiner states:

However, the products of Agrafiotis are equivalent to the products being claimed absent evidence to the contrary. Since no physical products are actually identified or produced in

the claims, the process limitations cannot be said to materially affect the nature of the product. The only apparent limitation in the claim that limits the nature of the molecules is that they could be made in a combinatorial synthesis of a reactant and a core. Therefore, Agrafiotis meets the limitations of the claims.

The examiner further notes that: "Applicant does not specifically address this rejection in the response." In reviewing applicants' last response, applicants appreciate the fact that a specific section response to the Agrafiotis rejection was not set forth. Applicants apologize for any confusion this may have caused. However, in the Remarks section applicants stated:

"Applicants would point out that the use of the validated descriptors places a limitation on the claimed molecules which are not known or anticipated by the prior art including Agrafiotis." May 25, 2004 response, page 20, end of 2nd full paragraph.

Applicants respectfully submit that based on the single fact alone that Agrafiotis does not teach or use validated molecular structural descriptors possessing a neighborhood property in his method, that Agrafiotis can not anticipate applicants' invention. Further, however, as more clearly reflected in the amended claims, applicants respectfully submit that the process limitations do materially affect the nature of the product. In claims 1 and 2, the molecules do not have similar three dimensional structures or activities. In claims 5 - 7, the molecules have three dimensional structures and activities similar to that of a lead compound. The molecules are restricted in their structure and activity in a way that Agrafiotis does not anticipate.

Applicants respectfully submit that the claims should no longer be rejected under 35 U.S.C. § 102(e).

Finally, Applicants have added new claims 8 – 12 which claim the set of molecules generated by the process recited in each claim and having the unique characteristics determined by that process.

Applicants respectfully submit that they have addressed and provided adequate responses to all the grounds of rejection raised by the examiner, and applicants respectfully request that the examiner remove the rejections of record and that a timely Notice of Allowance be issued in this case.

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Respectfully submitted,



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May 25, 2004 Response:

While the Examiner has characterized each rejection in accordance with the standards of the statutory section under which the rejection is based, there is a common thread that runs through and underlies all the rejections. Specifically, what appears to Applicants to be the problem is that the Examiner believes that, since there are no actual molecules described or molecular structures produced by the implemented processes, nothing substantive or useful is taught. Applicants respectfully disagree with the Examiner. What is taught in the patent and set forth in the claims are molecules which can be selected by a highly specific process from a vast universe of possible molecules which selected molecules share a specific useful characteristic. In particular, since molecular structural descriptors possessing a neighborhood property are used in

the process of selection, the molecules which are selected will all possess similar three dimensional shape characteristics which suggest that they will have a higher likelihood of possessing similar biological activity.

Applicants have amended the claims to more specifically characterize this useful feature of the invention and believe that with the amendments the problems cited by the Examiner under each basis of rejection are eliminated. The major amendments have been made to the claim preambles, and Applicants intend that the preambles be read as an integral part of the claims with the limitations recited in the preamble.

Applicants do not believe that claims directed to molecules having desired features in common must recite the specific molecular structures or families as long as it recites the specific method of identifying the molecules. *Note added: Perhaps the meaning of the sentence is clearer if it said: "...as long as it recites the specific method of characterizing the molecules and their relation to each other."*

A user of the methods described in claims 1-4 will select a molecule in which he/she is interested and which can be constructed from the information in the virtual library. The result of the use of the methods will result in a group of molecules (having similar three dimensional shapes and highly likely similar biological activities) which sample the molecular shape space which can be achieved using many different structural variations (reagents), cores, and chemistries. The group will not be oversampled. Applicants would point out that the use of the validated descriptors places a limitation on the claimed molecules which are not known or anticipated by the prior art including Agrafiotis.

Claims 5-7 identify molecules likely to have the same activity as a specific molecule known to the user. The claimed molecules will have similar shape (as characterized by the validated molecular structural descriptors possessing a neighborhood property) and likely biological activity out of all the possible molecules which could be formed from the structural variations, cores, and chemistries in the virtual library. Again, the identified molecules will not be oversampled.

Applicants respectfully submit that a person reasonably skilled in the art of computational chemistry will know how to use the invention to achieve the selection results for the specific molecules that person is interested in.